

(Cyclopentyloxy)acetic acid
95832-60-3 | DTXSID10538066

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

Model Results

Predicted value: 44.3 °C

Global applicability domain: Inside

Local applicability domain index: 6.81e-01

Confidence level: 5.47e-01

Nearest Neighbors from the Training Set

Image not found

3,3-Dimethyl-2-oxobutyric acid

Measured: 90.5

Predicted: 55.3

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2-Furanpropionic acid

Measured: 58.0

Predicted: 91.2

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Hexanoic acid, 5-oxo-

Measured: 13.5

Predicted: 29.1

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2-Ketoisovaleric acid

Measured: 31.5

Predicted: 32.6